SIMULATION AND TEST OF NANOCOMPOSITES FOR APPLICATION IN THE ARMY

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ABSTRACT

The purpose of this research is to simulate and test nanomaterial reinforced composites for potential applications in Army vehicles, especially for improved ballistic and blast protection. The resultant simulation and design system can address major concerns in functional requirements of nanomaterials in Army's ground vehicles such as strength, durability, ballistic and blast impact resistance. An important part of this research is to develop a comprehensive modeling tool to predict nano-composite behaviors. Based on a unit cell model developed for nanoclay-epoxy composites, the effect of nanomaterial distribution on the maximum stress developed in an epoxy resin was investigated by including modeling of the nanocaly-polymer interface. Tests were conducted on composite laminate/armor coupons that were reinforced by nanocomposites, including quasi-static mechanical tests, drop tower tests, shock tube tests, and ballistic tests. The ballistic tests indicate that armor with nanoclay insertion can survive more rounds of projectile impact. Shock tube tests showed that the damage in the laminate is less severe for samples with nanoclay reinforced epoxy resin than for those without nanoclay reinforcement. In addition, deflection was reduced about 43% with the usage of nanoclay reinforcement in the epoxy resin.

1. INTRODUCTION

Inspired by results obtained by Japanese researchers embedding nanoclay into nylon [1], extensive work has been carried out over the past 15 years on the incorporation of nanoclay into polymers for the purpose of enhancing the polymer properties. Normally the properties under investigation include tensile modulus, tensile strength, glass transition temperature, resistance against the absorption of moisture, resistance against flammability, and fracture toughness. It was found that the tensile modulus can be increased by 60% and tensile strength can be increased by 175%. Avila *et al*. [2] investigated the penetration mechanism on polymer-nanoclay-fiber glass nanocomposite using low-velocity impact tests (ASTM D5628-01). It was shown that the front side delamination area was reduced 22% by adding 1% nanoclay (by weight). Wetzel *et al*. [3] used a Charpy impact strength test to investigate the fracture toughness of nanocomposites. The addition of nano-particles is also beneficial to composite chemical and electrical properties. Numerical simulation for nanocomposites has also been a research focus in recent years. Hackett *et al*. [4] used Monte Carlo and molecular dynamics (MD) computer simulations to explore the atomic scale structure and dynamics of intercalated PEO-layered silicate nanocomposites. Instead of molecular-dynamics-based simulation method, Zhao and Hoa [5] examined tensile modulus, tensile strength and fracture toughness of a nanoclay reinforced epoxy cell using FEM simulation. It was shown that nano-particle volume percentage is the main factor for increased elastic modulus. Stress concentration in nanocomposite depends highly on the nano-particle dispersion. The more dispersive the nano-particle distribution, the less stress concentration exists in the composite. However, these models neglect the detailed characteristics of interface between nanoclay and epoxy, and are unable to account for effects of the interface properties. There exists a boundary layer near each nanoclay [6, 7],. The interphase region has different material properties from the bulk resin and nanofiller. Thus, it is important to model the interphase region to understand the nanocomposite property and to develop a modeling technique that analyzes the interface mechanical response of nanocomposites. Such a modeling approach would enable novel nanodevice design and multi-scale simulations of nanosystems. In this research, an interface element is developed for the simulation of nanoclay-polymer interface. Nanocomposite properties are simulated in a micro-scale unit cell. The obtained mechanical properties can then be used at the macro-scale for design optimization.

2. SIMULATIONS

A random sequential adsorption (RSA) schemes was used in this research to add nanoclays to a epoxy region by randomly generating the nanoclay location and orientation angle. A one-micron cell model was used in this research. At this size, the embedded nanoclay has appropriate length scale of 100-200 nanometers based on the SEM results. The insertion of nanoclays in the epoxy cell is illustrated in Fig. 1 (left). As can be seen, ten nanoclays

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14. ABSTRACT
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15. SUBJECT TERMS

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were added to the epoxy resin with 5 wt %. For each nanoclay insert, its layout is determined by the mid-point position, orientation angle, and the overall length. Another example of randomly distributed nanoclay with different weight percent is shown in Fig.1 (right). By using the computer program code developed, meshing for all the examples is generated easily.

2.1 Effect of nanoclay orientation on the properties of nano composite cell

One objective of this research is to study the effect of nano line orientation, using the developed modeling and simulation toolkit. The model has dimensions of 1000nm X 1000nm. Elongation (uniform displacement/length) of 5% of the 2-D cell model was considered. As shown in Fig. 2, the nodes along the bottom, marked with red, are constrained along Y direction. The nodes along the top, marked with green, have constrained displacement of 5% in the Y direction. Three cases were considered. With the same weight percent, nanoclays were distributed horizontally (case 1, top), vertically (case 2, middle), and randomly (case 3, bottom) in the epoxy. Material properties for epoxy resin and nanoclay are shown in Table 1.

Simulation results are presented in Figs. 2 and 3. As expected, there is stress concentration at the interface region, shown in Fig. 2. Load vs. displacement responses are shown in Fig.3. It can be seen that the stiffness for Case 1 is larger than the Case 2 and 3. It shows that the nanoclays reinforce the composite in Y direction, and the direction of nanoclay has a significant effect on the mechanical properties of nano composite.

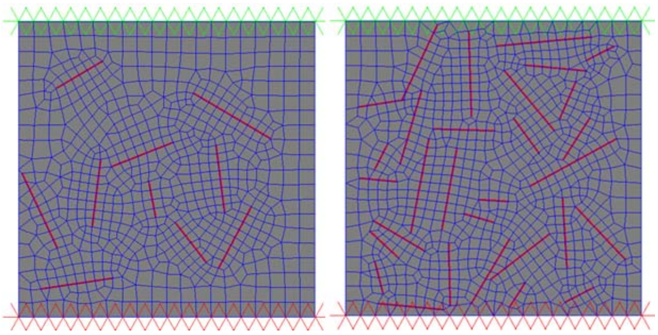


Figure 1 Nano composite unit cell with 5 wt % nanoclay (left) and 15 wt % nanoclay (right).

Table 1 Epoxy and nanoclay material in 2-D cell model

Items	Epoxy resin	Silicate Plate
Density (g/cm^3)	1.2	2.2
Modulus of elasticity (MPa)	2,300	73,000
Poisson's ratio	0.4	0.17
Tensile strength (MPa)	90	104

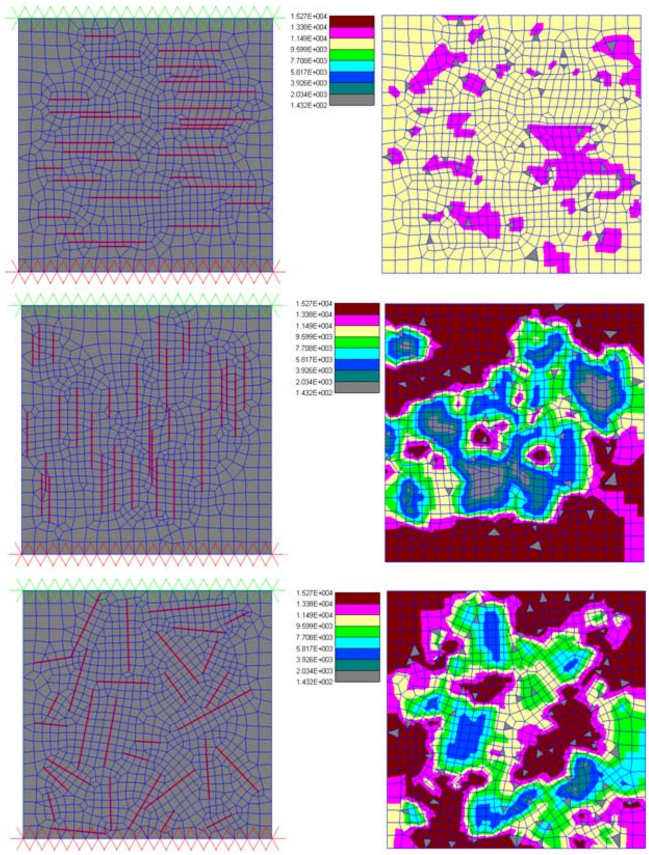


Figure 2 Nano composite unit cell with nanoclay distributed horizontally (top), vertically (middle), and randomly (bottom). Stress distributions in Y direction.

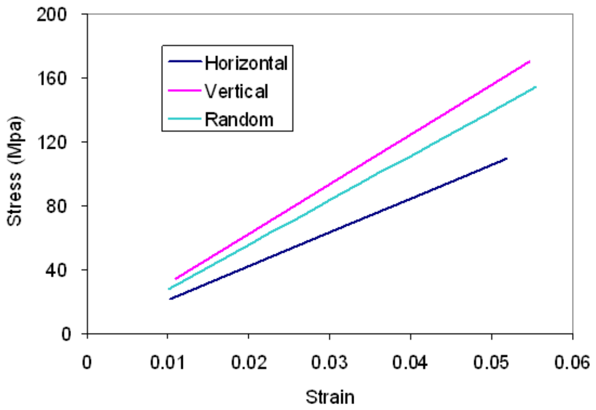


Figure 3 **C**omparison of stiffness of nano composite with nanoclay distributed horizontally, vertically, and randomly.

2.2 Interface elements in nano composite cell

An interface element was developed for the simulation of nanoclay-polymer interface. The interface formed by the element either has finite thickness (such as a replacement of adhesive layer in adhesive joints) or has zero thickness, such as delamination of composite laminates. Due to the small dimension of the boundary layer thickness, the nanoclay neighborhood was modeled by virtual nodes with zero thickness. The behavior of the interface element is defined by a traction-separation law. The crack is advanced, once a critical displacement or energy threshold is reached. In this study, the interface element was used to simulate the nano-composite with and without cracks along the interface.

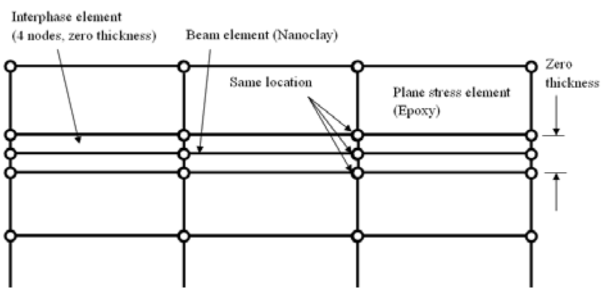


Figure 4 The strategy of interface element with zero thickness.

Figure 4 depicts the FEM strategy employed for nanocomposite interfaces. Four nodes elements with zero thickness are placed along the interface on both side of clay beam element, and they are used to connect the clay element and 2D plane-strain epoxy element. The system used in this study is for a general condition with both normal/opening and shear deformations, so called mixed-mode condition. Under mixed-mode loading, the interface element behavior is described by uncoupled opening and shear traction-separation laws. The energy release rate during the fracture process can be partitioned into two parts: opening (mode-I) and shear (mode-II). These two components are calculated by integrating the opening and shear traction-separation laws respectively:

$$\mathcal{G}_I = \int_0^{\delta_N} \sigma(\delta_N)d\delta_N\,; \qquad \mathcal{G}_{II} = \int_0^{\delta_T} \tau(\delta_T)d\delta_T \tag{1}$$

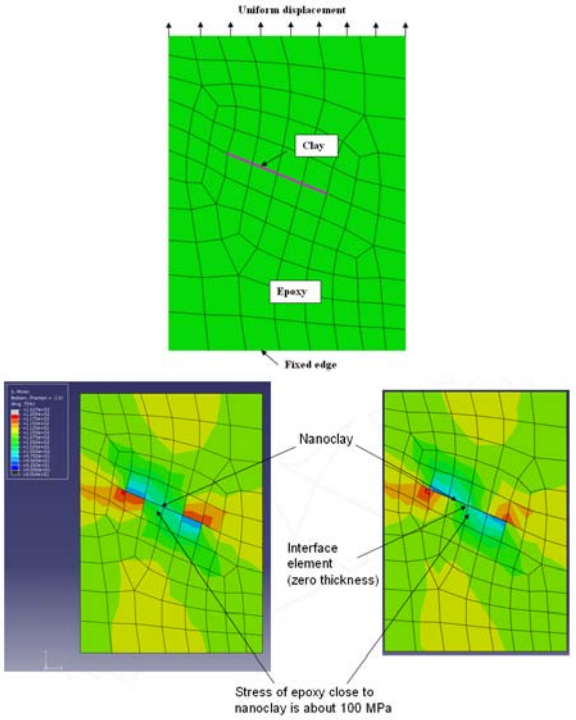
where δ_N and δ_T denote the relative normal and shear displacements. A linear interaction fracture criterion was adopted to predict the onset of fracture in this study:

$$G_I / \Gamma_I + G_{II} / \Gamma_{II} = 1 \tag{2}$$

where Γ_I and Γ_{II} are the total areas under the opening and shear traction-separation laws respectively. When the failure criterion of equation (2) is met, the element is assumed to fail and the crack advances by one element.

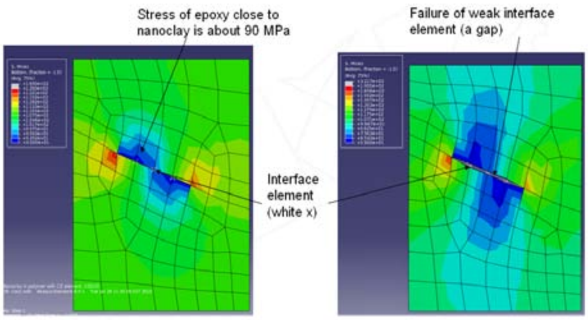
As the first example of a nanoclay-reinforced cell model with interface element, a simple case was studied to verify the FEM simulation. As shown in Fig. 4, a square cell of size one micron was investigated. One nanoclay is placed in the middle of epoxy. Material properties from Table 1 were used

Simulations with the interface element were performed using 3 different kinds of interface properties: Case I, strong interface element where the interface has the same properties as the nanoclay; Case II, medium-strong interface element where the interface has the similar properties as epoxy; and Case III, weak interface element where the interface has the lower properties than epoxy. The simulation results are shown in Fig.5 and Fig.6. Case I represents the no interface case, that is, a perfectly bonded condition between clay and epoxy. Therefore, comparison of results from Case 1 with a model that includes no interface at all can be used to verify that the interface element technique. As presented in Fig.5, both simulation results present a same stress distribution region.



(a) Without interface **(b) Case I**

Figure 5 Meshing of the nanoclay, interface and epoxy in FEM (top). FEM Simulation without interface element (bottom, left). FEM Simulation with interface element (Case I: strong element)



(c) Case II **(d) Case III**

Figure 6 FEM Simulation with interface element. Case II: intermediate and Case III: weak element.

In Case II, stress concentrations are present at interface region. However, since the interface properties is weaker, the stress concentration region is not as large as Case I. Furthermore, the stress in the epoxy is close to that of the nanoclay, about 90MPa, which is smaller than Case I (100 MPa). In Case III, as the interface properties are weaker than epoxy, there is gap/fracture observed at the interface region. Therefore it can be see that the interface between clay and epoxy has significant effect on the stress distribution.

3. EXPERIMENTS

3.1 Quasi-static tests and low velocity impact (LVI) tests

Nanocomposite samples were made for material tests, including static tests, low velocity impact tests, and Hopkinson bar impact tests. Samples are illustrated in Fig.7.

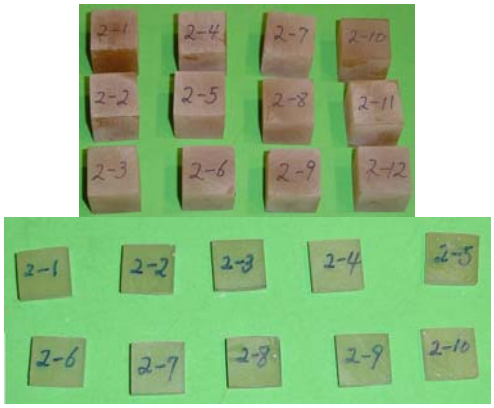
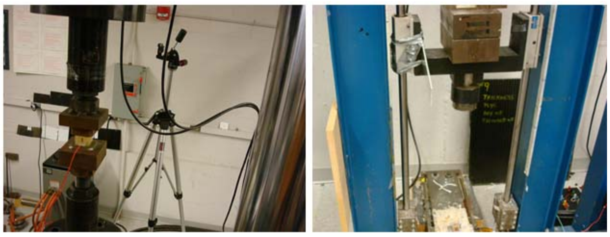


Figure 7 Test sample made of 5% nanoclay and epoxy. Cube-shaped nanoclay-epoxy samples (left). Nanoclay-epoxy sheets for Hopkinson Bar test for low-speed impact test (right).

Static tests and low-speed dynamic tests (drop tower tests) for epoxy with or without nanoclay reinforcement were performed. Nanoclay epoxy was seen to outperform pure epoxy. A decrease in Young's modulus and maximum stress were observed as the impact speed on the specimen increased. Compressive tests were performed on a servo-hydraulic machine for static tests. The experimental setup is shown in Fig. 8. Strain gage and load cell signals were recorded in each test. The axial cross-head movement rate imposed on the specimen was 0.010 mm/sec. Figure 9 shows the load-displacement results from compression tests for three pure epoxy and three nanoclay epoxy samples. For both groups, the load increased linearly up to a critical point where yield stress occurred. Subsequently, the load dropped and then increased until the maximum load capacity was reached. The corresponding Young's modulus, yield stress, maximum stress, and toughness are listed in Table 2. Here, fracture toughness (energy absorption during the loading process) is defined as the area under the load-displacement curve.

As can be seen from Table 2, the Young's modulus of epoxy with nanoclay is higher than that for pure epoxy. The average increase of Young's modulus is approximately 70% for nanoclay epoxy over pure epoxy.

This same trend can also be seen in the maximum stress values. The average maximum strength increased 5% for nanoclay-epoxy composite compared to the regular epoxy. However, nanoclay epoxy has a lower yield stress than pure epoxy. The average yield stress of nanoclay-epoxy mixture is 74 MPa, which is 16% lower than that of pure epoxy (90 MPa). Although the decrease of yield stress has a negative impact on nanoclay-epoxy under static load, the increased performance after yielding makes up for this loss in the static load case. In Fig. 9(right), the material strength increased rapidly until the maximum load capacity was reached. This stress hardening effect is similar to that of regular metallic materials, e.g., steel and aluminum. (NOTE: the stress hardening effect shown in Fig. 9(right) is limited by our load cell capacity. The real maximum stress would be even higher under higher loading conditions.)



(a) Static test (b) Dynamic test

Figure 8 Experimental setup for quasi-static compressive test (left) and LVI test (right).

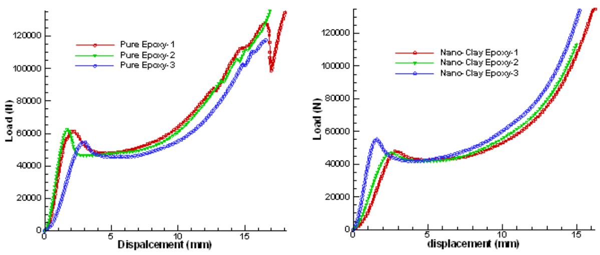


Figure 9 Load vs. displacement curves for quasi-static tests.

Table 2 Comparison of pure epoxy and nano-clay epoxy in static test

Specimen	Young's Modulus(GPa)	Yield Strength(MPa)	Max Strength(MPa)	Toughness (Joule)
Epoxy-1	2.02	91.5	189.8	1294
Epoxy-2	2.09	94.2	209.3	1135
Epoxy-3	1.91	81.8	174	971
Nano-Clay-Epoxy-1	3.84	70.9	198	907
Nano-Clay-Epoxy-2	2.88	69.9	169.6	792
Nano-Clay-Epoxy-3	3.56	82.3	233.4	1180

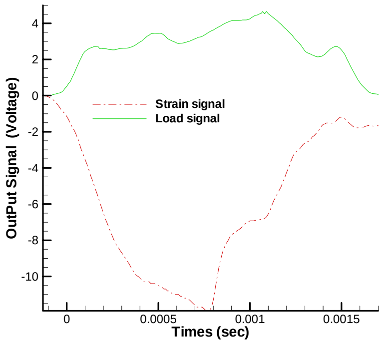


Figure 10 Typical load and strain signal for LVI tests.

Table 3 Dynamic tests for pure epoxy

Height	Young's Modulus(GPa)	Yield Strength(MPa)	Max Strength(MPa)	Toughness (Joule)
1.0m	1.31	95.9	153	635
1.0m	1.44	110	151	592
1.4m	0.745	88.4	88.4	169
1.4m	0.539	101	118	304

Table 4 Dynamic tests for nanoclay-epoxy

Height	Young's Modulus(GPa)	Yield Strength(MPa)	Max Strength(MPa)	Toughness (Joule)
1.0m	2.65	90.1	152	938
1.0m	2.38	87.5	132	654
1.4m	1.17	93	107	315
1.4m	1.37	107	113	318

Since the application of nanoclay-epoxy composite in armor relies more on a material's dynamic property, low-speed impact tests were performed using the drop tower as shown in Fig. 8. Two different drop heights of 1.0m, and 1.4m were chosen to study the strain rate effect on the properties of the specimens. For each drop height, two tests were performed. A strain gage on each specimen was connected to an oscilloscope. The load cell signal was used as the trigger signal for data acquisition. Figure 10 shows a typical response curve for the dynamic test. The positive curve is the signal for load cell. The negative curve is for the strain gage, under compression. From Fig. 10, it is seen that the load increases linearly at the beginning until a critical point, at which time the yield stress is defined. After yielding, a stress plateau is observed. Finally the load goes up again until the specimen loses its load capacity. This phenomenon was also observed in the static test (see Fig. 9).

The corresponding Young's modulus, yield stress, maximum stress, and toughness of the dynamic tests for pure epoxy and nanoclay epoxy are summarized in Tables 3 and 4. From Table 3, note that Young's modulus and maximum strength decrease as drop height increases. However, no obvious change of yield stress is observed. This finding is consistent with the static tests. That is,

Young's modulus and the maximum strength are higher in static tests than in dynamic tests. The experimental results of nano-clay epoxy in dynamic tests also show the same trend.

Comparison between pure epoxy and nanoclay epoxy in low-speed impact tests when drop height is fixed shows higher Young's modulus and maximum strength in nanoclay epoxy. At the drop height of 1.0 m, the average Young's modulus of nanoclay-epoxy specimen is 2.5 GPa, 79% higher than the modulus of pure epoxy. The average toughness of nanoclay-epoxy is 796 Joules, 30% higher than the toughness of pure epoxy. The yield stress and maximum stress of nanoclay-epoxy have no obvious improvement over pure epoxy. When the impact energy increases (drop height 1.4 m), the mechanical properties of all specimens decrease since the polymer based material has an impact softening effect. For nanoclay reinforced epoxy, the Young's modulus, yield stress, maximum stress, and toughness are 98%, 5.6%, 6.6%, and 34% higher than the counterparts of pure epoxy, respectively. The increase of mechanical properties of nanoclay-epoxy composite demonstrates the advantage of embedding nanoclay particles in epoxy resin.

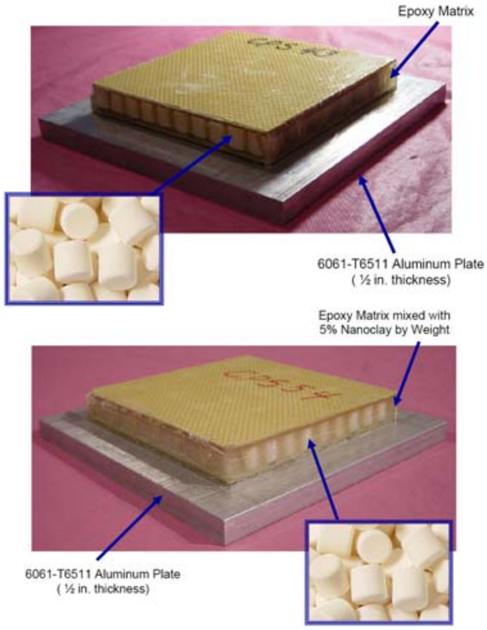
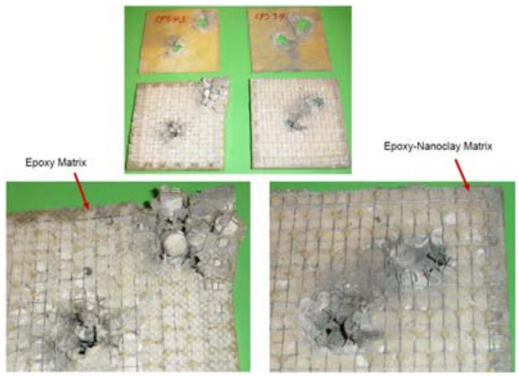


Figure 12 Armor samples with pure epoxy (top) and epoxy with 5% nanoclay (bottom).

3.2 Ballistic tests on nanoclay reinforced nano composite laminate

Ballistic tests were carried out for composite armor coupons that use nanocomposites. The general construction of the composite armor is shown in Fig. 12. Each armor sample is composed of an aluminum backplate and a ceramic face plate. The face plate is a combination of ceramic pellet and gluing polymer. The gluing polymer is pure epoxy or nanoclay reinforced epoxy. The projectiles used in the ballistic test were APM2 and B32 bullets. Each test armor sample was shot by an APM2 bullet first, then the B32 bullet. The armor was checked after the two rounds for damage assessment.



(a) Damage of the ceramic face plates

(b) The top surface damage of back plates

(c) The bottom surface damage of back plates

Figure 13 Comparison of ballistic test results.

Figure 12 shows two armor samples used in the nanocomposite performance check. The armor in Fig. 12(top) used pure epoxy in the face plate, while the armor in Fig. 12(bottom) used epoxy with 5% nanoclay in the face plate. Both armors in Fig. 12 had the same geometry configuration, ceramic material, and back plate, so the 5% nanoclay reinforcement was the only difference between the two armors. The ballistic test results are shown in Fig. 13. After two rounds, the armor with nanoclay insertion still maintained the face plate integrity (see Fig. 13a), which indicates the armor with nanoclay can withstand more rounds of projectile impact. Similar conclusions can be deduced from the back plate damage (Figs. 13b and 13c). The nanoclay reinforced armor shows better impact resistance.

3.3 Shock tube tests on nanoclay reinforced nano composite

Blast tube tests were conducted. The test bench is shown in Fig. 11. Four channels of response signals were recorded. They are located on the blast tube for blast overpressure determination and on the back plate of test samples for maximum deformation. One representative set of response signals is displayed in Fig. 15.

The test samples for the blast tube test are shown in Fig. 16. There are three groups of test samples: fiberglass laminate, carbon fiber laminate, and the para-aramid fiber laminate. Two bonding media are used for comparison, including pure epoxy and the nanoclay-reinforced epoxy.

The dimension of the test samples are listed in Table 4. The length of each sample panel is approximately 6 inch. The fiberglass laminate is the heaviest sample among all the samples, while the para-aramid fiber laminate is slightly lighter than the carbon fiber laminate.

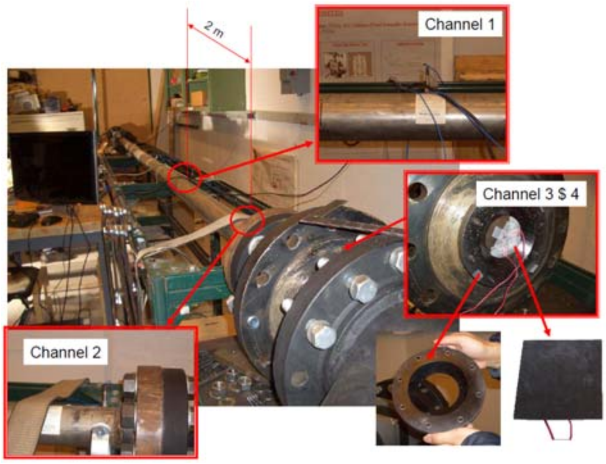


Figure 14 Blast tube test bench.

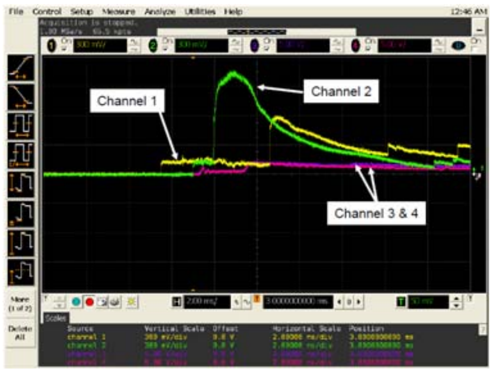


Figure 15 Response signals from the blast tube test

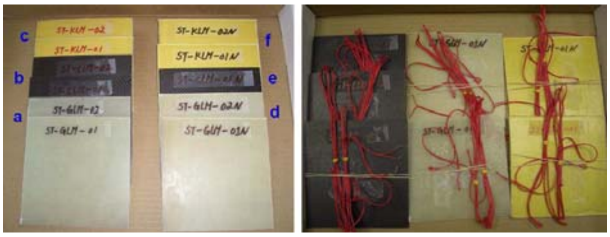


Figure 16 Test samples for the blast tube test

Figure 17 shows the comparison of carbon fiber laminates from the blast tube tests. The peak pressure in the blast tube was approximately 610 psi. The damage in the laminate is less severe for the sample with nanoclay-reinforced epoxy resin than the damage in the sample made of pure epoxy resin. Damage of the para-aramid fiber laminate samples is observed in Fig. 18. The diameter of the shock wave impact surface is about 78 mm. The maximum deflection of the laminate plate is compared: 5.1 mm for pure epoxy resin, and 2.9 mm for nanocomposite resin. As can be seen, the deflection reduction is about 43% with the usage of nanoclay reinforcement in the epoxy resin.

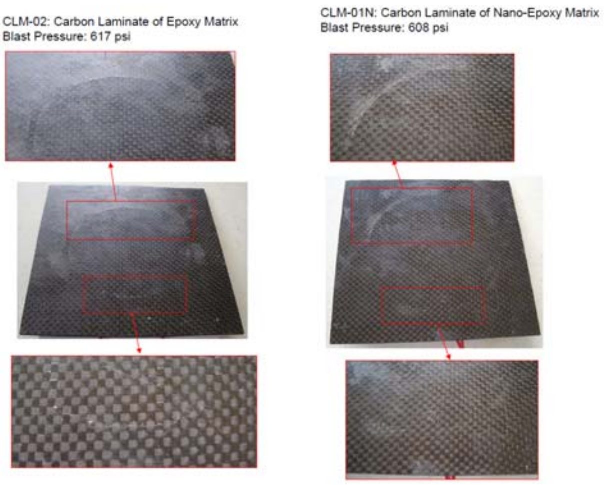


Figure 17 Comparison of test results for carbon fiber laminates with pure epoxy resin (left) and nanoclay-reinforced epoxy resin (right).

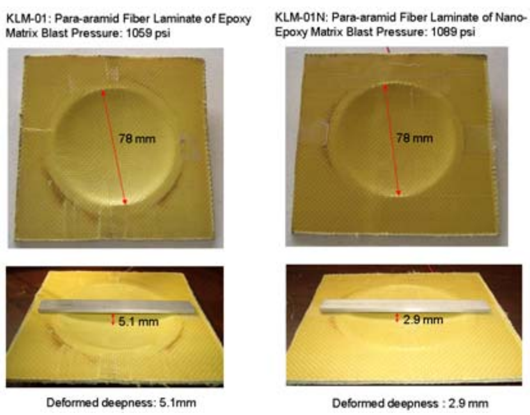


Figure 18 Comparison of test results for para-aramid fiber laminates.

CONCLUSIONS

A comprehensive modeling tool to predict nano-composite behaviors has been developed for simulation of nanoclay-epoxy composites. The effect of nanomaterials distribution on the maximum stress developed in epoxy resin was investigated by including the simulation of nanocaly-polymer interface. Experimental results for quasi-static mechanical tests, drop tower tests, shock tube tests, and ballistic tests for composite laminate/armor reinforced by nanocomposites were presented. The results from ballistic tests indicate that the armor with nanoclay insertion can withstand more rounds of projectile impact. The shock tube tests show that the damage in the laminate is less severe for samples with nanoclay reinforced epoxy resin than those without nanoclay reinforcement. These results demonstrate the promise of including nanocomposite systems on Army vehicles for enhanced ballistic and blast protection.

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